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A note of Zagreb indices of nanostar dendrimers

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The Zagreb indices have been introduced more than thirty years ago by Gutman and Trinajstić. In this paper we introduce a new version of Zagreb indices and then we compute them for an infinite family of nanostar dendrimers.

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1. Introduction

A graph is a collection of points and lines connecting a subset of them. The points and lines of a graph also called vertices and edges of the graph, respectively. If e is an edge of G, connecting the vertices u and v, then we write $e = uv$ and say "u and v are adjacent". A connected graph is a graph such that there is a path between all pairs of vertices. A molecular graph is a simple graph such that its vertices correspond to the atoms and the edges to the bonds. Note that hydrogen atoms are often omitted.

Let Σ be the class of finite graphs. A topological index is a function $Top : \Sigma \to R^{\geq 0}$ with this property that $Top(G) = Top(H)$, if G and H are isomorphic.

The Zagreb indices have been introduced more than 30 years ago by Gutman and Trinajstić[7]. They are defined as:

$$M_1(G) = \sum_{v\in V(G)} (d_G(v))^2 \text{ and}$$

$$M_2(G) = \sum_{uv\in E(G)} d_G(u)d_G(v)\ .$$

Now we define a new version of Zagreb indices as follows:

$$M_1'(G) = \sum_{uv\in E(G)} \delta_G(u) + \delta_G(v) \text{ and}$$

$$M_2'(G) = \sum_{uv\in E(G)} \delta_G(u)\delta_G(v)\ .$$

where $\delta_G(u) = \sum_{v\in N_G(u)} d_G(v)$ and $N_G(u) = \{v \in V(G) \mid uv \in E(G)\}$. One can see that $M_1'(G) = \sum_{u\in V(G)} d_G(u)\delta_G(u)$.

This paper addresses the problem of computing the the new Zagreb indices of a special type of dendrimers. We encourage the readers to consult papers [8 - 11] for computational techniques related to dendrimers, as well as [12 - 26] for background materials. Our notation is standard and taken mainly from the standard books of graph theory such as [15].

2. Main results and discussion

The aim of this paper is computing the new version of Zagreb indices of a class of dendrimers. To do this, let $U = \{u_1, u_2, \ldots, u_k\}$ be a subset of $V(G)$. The *truncated Zagreb indices* $M_1'^{(U)}(G)$ and $M_2'^{(U)}(G)$ can be defined as

$$M_1'^{(U)}(G) = M_1'^{(u_1,u_2,\ldots,u_k)}(G) = \sum_{u\in V(G)-U} d_G(u)\delta_G(u)$$

and

$$M_2'^{(U)}(G) = M_2'^{(u_1,u_2,\ldots,u_k)}(G) = \sum_{\substack{uv\in E(G)\\ u,v\notin U}} \delta_G(u)\delta_G(v)$$

It should be noticed that in the case $U = \emptyset$, $M_1'^{(U)}(G) = M_1'(G)$ and $M_2'^{(U)}(G) = M_2'(G)$.

Let G_i $(1 \leq i \leq n)$ be some graphs and $v_i \in V(G_i)$. A chain graph denoted by $G = G(G_1, \ldots, G_n, v_1, \ldots, v_n)$ is obtained from the union of the graphs G_i, $i = 1, 2, \ldots, n$, by adding the edges v_iv_{i+1} $(1 \leq i \leq n-1)$, see Fig. 2. Then $|V(G)| = \sum_{i=1}^{n} |V(G_i)|$ and $|E(G)| = (n-1) + \sum_{i=1}^{n} |E(G_i)|$.

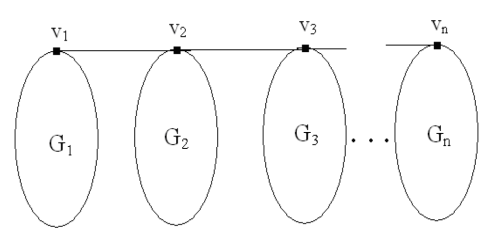

Fig. 1. The chain graph $G = G(G_1, \ldots, G_n, v_1, \ldots, v_n)$.

It is worth noting that the above specified class of chain graphs embraces, as special cases, all trees (among which are the molecular graphs of alkanes) and all unicyclic graphs (among which are the molecular graphs of monocycloalkanes). Also the molecular graphs of many polymers and dendrimers are chain graphs.

Lemma 1. Suppose that $G = G(G_1, G_2, ..., G_n, v_1, v_2, ..., v_n)$ is a chain graph and $N_G[u] = N_G(u) \cup \{u\}$. Then:

(i) $G(G_1, G_2, ..., G_n, v_1, v_2, ..., v_n)$ is connected if and only if G ($1 \le i \le n$) are connected.

(ii) $$\mathrm{d}_G(a) = \begin{cases} \mathrm{d}_{G_i}(a) & a \in V(G_i) \text{ and } a \ne v_i \\ \mathrm{d}_{G_i}(a)+1 & a = v_i,\ i = 1, n \\ \mathrm{d}_{G_i}(a)+2 & a = v_i,\ 2 \le i \le n-1 \end{cases}.$$

(iii) if $u \in V(G)$ and $v_i \notin N_{G_i}[u]$ then $\delta_G(u) = \delta_{G_i}(u)$.

Theorem 2. If $n \ge 2$ and $v_1, ..., v_n \ne u_1, ..., u_k$, then for $G = G(G_1, G_2, ..., G_n, v_1, v_2, ..., v_n)$ it holds:

$$M_1'^{(U)}(G) = \sum_{i=1}^{n} M_1'^{(U)}(G_i) + 4\sum_{i=2}^{n-1} \delta_{G_i}(v_i) + 2\sum_{i=1,n} \delta_{G_i}(v_i) + \sum_{i=2}^{n-1}\left(d_{G_i}(v_i)+2\right)\left(d_G(v_{i-1})+d_G(v_{i+1})\right) + \left(d_{G_1}(v_1)+1\right)d_G(v_2) + \left(d_{G_n}(v_n)+1\right)d_G(v_{n-1}).$$

Proof. By using the definition of the truncated M_1' index one can see that

$$\begin{aligned} M_1'^{(U)}(G) &= \sum_{u \in V(G)-U} d_G(u)\delta_G(u) \\ &= \sum_{\substack{u \in V(G)-U \\ u \notin \bigcup_{i=1}^{n} N_{G_i}[v_i]}} d_G(u)\delta_G(u) + \sum_{\substack{u \in V(G)-U \\ u \in \bigcup_{i=1}^{n} N_{G_i}[v_i]}} d_G(u)\delta_G(u) \\ &= \sum_{i=1}^{n} M_1'^{\left(U \cup N_{G_i}[v_i]\right)}(G_i) + \sum_{i=2}^{n-1} \sum_{v \in N_{G_i}[v_i]-U} d_{G_i}(v)\left(\delta_{G_i}(v)+2\right) \\ &\quad + \sum_{i=1,n} \sum_{v \in N_{G_i}[v_i]-U} d_{G_i}(v)\left(\delta_{G_i}(v)+1\right) \\ &\quad + \sum_{i=2}^{n-1}\left(\delta_{G_i}(v_i)+2\right)\left(\delta_{G_i}(v_i)+d_G(v_{i-1})+d_G(v_{i+1})\right) \\ &\quad + \left(d_{G_1}(v_1)+1\right)\left(\delta_{G_1}(v_1)+d_G(v_2)\right) \\ &\quad + \left(d_{G_n}(v_n)+1\right)\left(\delta_{G_n}(v_n)+d_G(v_{n-1})\right) \\ &= \sum_{i=1}^{n} M_1'^{(U)}(G_i) + 4\sum_{i=2}^{n-1} \delta_{G_i}(v_i) + 2\sum_{i=1,n} \delta_{G_i}(v_i) \\ &\quad + \sum_{i=2}^{n-1}\left(d_{G_i}(v_i)+2\right)\left(d_G(v_{i-1})+d_G(v_{i+1})\right) + \left(d_{G_1}(v_1)+1\right)d_G(v_2) \\ &\quad + \left(d_{G_n}(v_n)+1\right)d_G(v_{n-1}). \end{aligned}$$

Corollary 3. The truncated M_1' index of the chain graph $G = G(G_1, G_2, v_1, v_2)$ ($v_1, v_2 \ne u_1, ..., u_k$) is:

$$M_1'(G) = \sum_{i=1}^{2} M_1'(G_i) + 2\left(\delta_{G_1}(v_1)+\delta_{G_2}(v_2)\right) + 2\left(d_{G_1}(v_1)+1\right)\left(d_{G_2}(v_2)+1\right).$$

We use from this corollary in the next section.

Theorem 4. If $n \ge 2$ and $v_1, ..., v_n \ne u_1, ..., u_k$, then for $G = G(G_1, G_2, ..., G_n, v_1, v_2, ..., v_n)$ it holds:

$$M_2'^{(U)}(G) = \sum_{i=1}^{n} M_2'^{\left(U \cup N_{G_i}[v_i]\right)}(G_i) + \sum_{i=1}^{n} \sum_{\substack{uv \in E(G_i) \\ u \in N_{G_i}[v_i] \\ u,v \notin U}} \delta_G(u)\delta_G(v) + \sum_{i=1}^{n-1} \delta_G(v_i)\delta_G(v_{i+1}).$$

Proof. By using the definition of the truncated M_2' index one can see that

$$\begin{aligned} M_2'^{(U)}(G) &= \sum_{\substack{uv \in E(G) \\ u,v \notin U}} \delta_G(u)\delta_G(v) \\ &= \sum_{\substack{uv \in E(G) \\ u,v \notin \bigcup_{i=1}^{n} N_{G_i}[v_i] \cup U}} \delta_G(u)\delta_G(v) + \sum_{\substack{uv \in E(G) \\ u \in \bigcup_{i=1}^{n} N_{G_i}[v_i] \\ u,v \notin U}} \delta_G(u)\delta_G(v) \\ &= \sum_{i=1}^{n} M_2'^{\left(U \cup N_{G_i}[v_i]\right)}(G_i) + \sum_{i=1}^{n} \sum_{\substack{uv \in E(G_i) \\ u \in N_{G_i}[v_i] \\ u,v \notin U}} \delta_G(u)\delta_G(v) \\ &\quad + \sum_{i=1}^{n-1} \delta_G(v_i)\delta_G(v_{i+1}). \end{aligned}$$

Corollary 5. The truncated M_2' index of the chain graph $G = G(G_1, G_2, v_1, v_2)$ ($v_1, v_2 \ne u_1, ..., u_k$) is:

$$M_2'(G)=\sum_{i=1}^{2} M_2'^{\left(N_{G_i}[v_i]\right)}(G_i)\ +$$
$$\sum_{i=1}^{2}\sum_{\substack{uv\in E(G_i)\\ u\in N_{G_i}[v_i]}} \delta_G(u)\delta_G(v)$$
$$+\ \left(\delta_{G_1}(v_1)+d_{G_2}(v_2)+2\right)\left(\delta_{G_2}(v_2)+d_{G_1}(v_1)+2\right).$$

We use from this corollary in the next section too.

Example 6. Consider the graph G_1 shown in Fig. 2. It is easy to see that

$$M_1'(G_1)=222 \text{ and } M_2'(G_1)=615,$$
$$M_2'^{(N_{G_1}[v_1])}(G_1)=M_2'^{(N_{G_1}[v_2])}(G_1)$$
$$=M_2'^{(N_{G_1}[v_3])}(G_1)=M_2'^{(N_{G_1}[v])}(G_1)=543$$

and so, for $1\le i,j\le 3, i\ne j$,

$$M_2'^{(N_{G_1}[v_i]\cup N_{G_1}[v_j])}(G_1)=471.$$

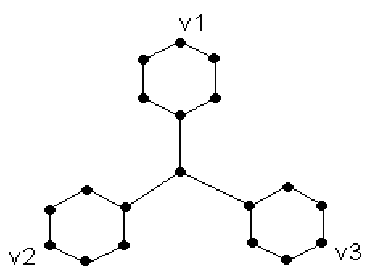

Fig. 2. The graph of nanostar G_n for n=1.

Consider now the chain graph $G_n=G(G_{n-1},H_1,v_1,u_1)$, shown in Fig. 2 (for $n=1$) and Figure 3, respectively. It is easy to see that $H_i\cong G_1$ ($1\le i\le n-1$) and

$$G_n=G(G_{n-1},H_1,v_1,u_1)$$
$$G_{n-1}=G(G_{n-2},H_2,v_2,u_2)$$
$$\vdots$$
$$G_{n-i}=G(G_{n-i-1},H_{i+1},v_{i+1},u_{i+1})$$
$$\vdots$$
$$G_2=G(G_1,H_{n-1},v_{n-1},u_{n-1}).$$

Then by using corollary 3, we have the following relations:

$$M_1'(G_n)=M_1'(G_{n-1})+M_1'(H_1)+34$$
$$M_1'(G_{n-1})=M_1'(G_{n-2})+M_1'(H_2)+34$$
$$\vdots$$
$$M_1'(G_{n-i})=M_1'(G_{n-i-1})+M_1'(H_{i+1})+34$$
$$\vdots$$
$$M_1'(G_2)=M_1'(G_1)+M_1'(H_{n-1})+34.$$

Summation of these relations yields

$$M_1'(G_n)=M_1'(G_1)+\sum_{i=1}^{n-1}M_1'(H_i)+34(n-1),$$

it is easy to obtain

$$M_1'(G_n)=nM_1'(G_1)+34(n-1)=256n-34.$$

On the other word by using corollary 5, we have the following relations:

$$M_2'(G_n)=M_2'^{\left(N_{G_{n-1}}[v_1]\right)}(G_{n-1})\ +$$
$$M_2'^{\left(N_{H_1}[u_1]\right)}(H_1)+289$$

$$M_2'^{\left(N_{G_{n-1}}[v_1]\right)}(G_{n-1})=M_2'^{\left(N_{G_{n-2}}[v_2]\right)}(G_{n-2})\ +$$
$$M_2'^{\left(N_{H_2}[v_1]\cup N_{H_2}[u_2]\right)}(H_2)+289$$
$$\vdots$$
$$M_2'^{\left(N_{G_{n-i}}[v_i]\right)}(G_{n-i})=M_2'^{\left(N_{G_{n-i-1}}[v_{i+1}]\right)}(G_{n-i-1})\ +$$
$$M_2'^{\left(N_{H_{i+1}}[v_i]\cup N_{H_{i+1}}[u_{i+1}]\right)}(H_{i+1})+289\ \vdots$$
$$M_2'^{\left(N_{G_2}[v_{n-2}]\right)}(G_2)=M_2'^{\left(N_{G_1}[v_{n-1}]\right)}(G_1)\ +$$
$$M_2'^{\left(N_{H_{n-1}}[v_{n-2}]\cup N_{H_{n-1}}[u_{n-1}]\right)}(H_{n-1})+289.$$

Summation of these relations yields

$$M_2'(G_n)=M_2'^{\left(N_{G_1}[v_{n-1}]\right)}(G_1)+M_2'^{\left(N_{H_1}[u_1]\right)}(H_1)$$
$$+\sum_{i=2}^{n-1}M_2'^{\left(N_{H_i}[v_{i-1}]\cup N_{H_i}[u_i]\right)}(H_i)+289(n-1),$$

it is easy to obtain

$$M_2'(G_n)=2M_2'^{\left(N_{G_1}[v_1]\right)}(G_1)\ +$$
$$(n-2)M_2'^{\left(N_{G_1}[v_1]\cup N_{G_1}[v_2]\right)}(G_1)+289(n-1)$$
$$=760n-145.$$

In other words we arrived at the following:

Theorem 7. Consider the chain graph $G_n=G(G_{n-1},H_1,v_1,u_1)$ $(n\ge 2)$, shown in Fig. 3. Then,

$$M_1'(G_n)=256n-34$$

And

$$M_2'(G_n)=760n-145.$$

Corollary 8. Consider the nanostar dendrimer D, shown in Fig. 4. Then,

$$M_1'(D)=256n-34 \text{ and } M_2'(D)=760n-145,$$

where *n* is the number of repetition of the fragment G_1.

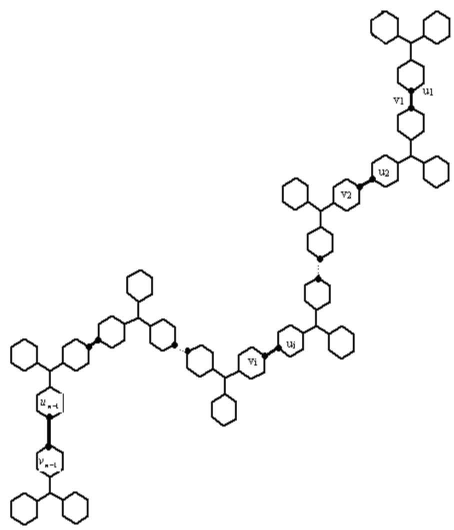

Fig. 3. The chain graph G_n and the labeling of its vertices.

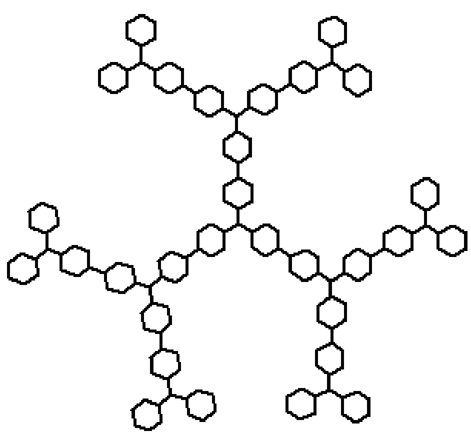

Fig. 4. The graph of the nanostar dendrimer D.

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